

CRYSTALLOGRAPHIC AND GEODESIC RADON TRANSFORMS ON $SO(3)$: MOTIVATION, GENERALIZATION, DISCRETIZATION

Dedicated to S. Helgason on his 85-th Birthday

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1. INTRODUCTION

In this paper we consider the so-called crystallographic Radon transform (or crystallographic X -ray transform) and totally geodesic Radon transform on the group of rotations $SO(3)$. As we show both of these transforms naturally appear in texture analysis, i.e. the analysis of preferred crystallographic orientation. Although we discuss only applications to texture analysis both transforms have other applications as well.

In section 2 we start with motivations and applications. In sections 3 and 4 we develop a general framework on compact Lie groups. In section 5 we give a detailed analysis of the totally geodesic Radon transform on $SO(3)$. In section 6 we compare crystallographic Radon transform on $SO(3)$ and Funk transform on S^3 . In section 7 we show non-invertibility of the crystallographic transform. In section 8 we describe an *exact* reconstruction formula for bandlimited functions, which uses only a *finite* number of samples of their Radon transform. Some auxiliary results for this section are collected in Appendix.

The Radon transform on $SO(3)$ has recently attracted attention of many mathematicians. In addition to articles, which will be mentioned in our paper later we also refer to [5], [15], [16], [17], [21], [22].

2. TEXTURE GONIOMETRY

A first mathematical description of the inversion problem in texture analysis was given in [6] and [7]. Let us recall the basics of texture analysis and texture goniometry (see [3] and [4]). Texture analysis is the analysis of the statistical distribution of orientations of crystals within a specimen of a polycrystalline material, which could be metals or rocks. A crystallographic

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orientation is a set of crystal symmetrically equivalent rotations between an individual crystal and the specimen.

The orientation distribution by volume requires a measure of the volume portion $\Delta V/V$ of a polycrystalline specimen of total volume V carrying crystal grains with orientations within a volume element $\Delta G \subset G$ of the subgroup G of all feasible $G \in SO(3)$.

The orientation g of an individual crystal is the active rotation $g \in SO(3)$ that maps a right-handed orthonormal co-ordinate system fixed to the specimen onto another right-handed orthonormal co-ordinate system fixed to the crystal. In other words if a unit direction is represented by unit vectors h with respect to the crystal frame where as the same direction is represented by the vector r with respect to the specimen frame then $h = gr$.

Assuming that the measure possesses a probability density function $f : G \rightarrow \mathbb{R}_+$, then

$$\text{prob}(g \in \Delta G) = \int_{\Delta G} f(g) d\omega_g$$

and f is referred to as the *orientation density function* (ODE) by volume and the Riemannian measure on S^3 is

$$d\omega_g = \sin \beta d\alpha d\beta d\gamma,$$

where α, β, γ are the Euler angles. Note that $d\omega_g = 8\pi^2 dg$, where dg is the invariant Haar measure on $SO(3)$.

In X-ray diffraction experiments, the orientation density function f cannot be directly measured but with a texture goniometer the *pole density function* (PDF) $P(h, r)$ can be sampled. $P(h, r)$ represents that a fixed crystal direction h or its antipodal $-h$ statistically coincides with the specimen direction r due to Friedel's law in crystallography [10]. The PDF or *crystallographic X-ray transform* is the tomographic projection of an orientation density function given by the formula

$$(1) \quad Pf(h, r) = \frac{1}{2}(\mathcal{R}f(h, r) + \mathcal{R}f(-h, r)),$$

where the *Radon transform* is defined as

$$(2) \quad \begin{aligned} (\mathcal{R}f)(h, r) &= \frac{1}{2\pi} \int_{\{g \in SO(3) : h = gr\}} f(g) d\omega_g = \\ 4\pi \int_{SO(3)} f(g) \delta_r(g^{-1}h) dg &= (f * \delta_r)(h), \quad (h, r) \in S^2 \times S^2, \end{aligned}$$

where δ_r is the measure concentrated on the set of all $g \in SO(3)$ such that $h = gr$.

Since ODF f is a probability density it has to have the following properties:

- (a) $f(g) \geq 0, \quad h, r \in S^2,$
- (b) $\int_{SO(3)} f(g) dg = 1.$

In what follows we will discuss inversion of crystallographic X -ray transform Pf and Radon transform $\mathcal{R}f$.

First we formulate what can be called analytic reconstruction problems.

Problem 1. *Reconstruct the ODF $f(g)$, $g \in SO(3)$, from PDF $Pf(h, r)$, $h, r \in S^2$.*

It will be shown in section 7 that this problem is unsolvable in general since the mapping

$$f \rightarrow Pf$$

has non-trivial kernel.

Problem 2. *Reconstruct $f(g)$, $g \in SO(3)$, from all $\mathcal{R}f(h, r)$, $h, r \in S^2$.*

An explicit solution to this problem will be given in section 5.

In practice only a finite number of pole figures $P(h, r)$, $h, r \in S^2$, can be measured. Therefore the real life reconstruction problem is the following.

Problem 3. *Using a finite number of pole figures $P(h_i, r_j)$, $h_i, r_j \in S^2$, $i = 1, \dots, n$, $j = 1, \dots, m$, find a function f on $SO(3)$, which would satisfy (in some sense) equations (1) and (2) and conditions (a) and (b).*

An approximate solution to this problem, which is described in terms of Gabor frames was found in [8].

The corresponding discrete problem for $\mathcal{R}f$ can be formulated as follows.

Problem 4. *Reconstruct $f(g)$, $g \in SO(3)$, from a finite number of samples $\mathcal{R}f(h_j, r_j)$, $h_j, r_j \in S^2$, $j = 1, \dots, m$.*

This problem will be solved in section 8 for bandlimited functions on $SO(3)$. We were able to obtain an *exact* reconstruction formula for bandlimited functions, which uses only a *finite* number of samples of their Radon transform.

In section 4 we extend Problem 2 to general compact Lie groups. Namely, we consider the following problem.

Problem 5. *Let \mathcal{H} be a subgroup of the compact Lie group \mathcal{G} . Determine domain and range for the Radon transform*

$$\mathcal{R}f(x, y) = \int_{\mathcal{H}} f(xhy^{-1}) dh, \quad x, y \in \mathcal{G}.$$

In section 3 we remind basic facts about Fourier analysis on compact Lie groups. In section 6 we compare crystallographic X -ray transform on $SO(3)$ and Funk transform on S^3 . In Appendix 9 we briefly explain major ingredients of the proof of our Discrete Inversion Formula in section 8.

3. FOURIER ANALYSIS ON COMPACT GROUPS

Let \mathcal{G} be a compact Lie group. A unitary representation of \mathcal{G} is a continuous group homomorphism $\pi: \mathcal{G} \rightarrow U(d_\pi)$ of \mathcal{G} into the group of unitary matrices of a certain dimension d_π . Such a representation is irreducible if

$\pi(g)M = M\pi(g)$ for all $g \in \mathcal{G}$ and some $M \in \mathbb{C}^{d_\pi \times d_\pi}$ implies $M = cI$, where I is the identity matrix. Equivalently, \mathbb{C}^{d_π} does not have non-trivial π -invariant subspaces $V \subset \mathbb{C}^{d_\pi}$ with $\pi(g)V \subset V$ for all $g \in \mathcal{G}$. Two representations π_1 and π_2 are equivalent, if there exists an invertible matrix M such that $\pi_1(g)M = M\pi_2(g)$ for all $g \in \mathcal{G}$.

Let $\hat{\mathcal{G}}$ denote the set of all equivalence classes of irreducible representations. This set parameterizes an orthogonal decomposition of the Hilbert space $L^2(\mathcal{G})$ constructed with respect to the normalized Haar measure.

Theorem 1 (Peter-Weyl, [28]). *Let \mathcal{G} be a compact Lie group. Then the following statements are true.*

a: Denote $H_\pi = \{g \mapsto \text{trace}(\pi(g)M) : M \in \mathbb{C}^{d_\pi \times d_\pi}\}$. Then the Hilbert space $L^2(\mathcal{G})$ decomposes into the orthogonal direct sum

$$(3) \quad L^2(\mathcal{G}) = \bigoplus_{\pi \in \hat{\mathcal{G}}} H_\pi$$

b: For each irreducible representation $\pi \in \hat{\mathcal{G}}$ the orthogonal projection $L^2(\mathcal{G}) \rightarrow H_\pi$ is given by

$$(4) \quad f \mapsto d_\pi \int_{\mathcal{G}} f(h) \chi_\pi(h^{-1}g) dh = d_\pi f * \chi_\pi,$$

in terms of the character $\chi_\pi(g) = \text{trace}(\pi(g))$ of the representation and dh is the normalized Haar measure.

We will denote the matrix M in the equation $f * \chi_\pi = \text{trace}(\pi(g)M)$ as Fourier coefficient $\hat{f}(\pi)$ of f at the irreducible representation π . The Fourier coefficient can be calculated as

$$\hat{f}(\pi) = \int_{\mathcal{G}} f(g) \pi^*(g) dg.$$

The inversion formula (the Fourier expansion) is then given by

$$f(g) = \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \text{trace}(\pi(g) \hat{f}(\pi)).$$

If we denote by $\|M\|_{HS}^2 = \text{trace}(M^*M)$ the Frobenius or Hilbert-Schmidt norm of a matrix M , then the following Parseval identity is true.

Proposition 1 (Parseval identity). *Let $f \in L^2(\mathcal{G})$. Then the matrix-valued Fourier coefficients $\hat{f} \in \mathbb{C}^{d_\pi \times d_\pi}$ satisfy*

$$(5) \quad \|f\|^2 = \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \|\hat{f}(\pi)\|_{HS}^2.$$

On the group \mathcal{G} one defines the convolution of two integrable functions $f, r \in L^1(\mathcal{G})$ as

$$f * r(g) = \int_{\mathcal{G}} f(h) r(h^{-1}g) dh.$$

Since $f * r \in L^1(\mathcal{G})$, the Fourier coefficients are well-defined and they satisfy

Proposition 2 (Convolution theorem on \mathcal{G}). *Let $f, r \in L^1(\mathcal{G})$ then $f * r \in L^1(\mathcal{G})$ and*

$$\widehat{f * r}(\pi) = \hat{f}(\pi)\hat{r}(\pi).$$

The group structure gives rise to left and right translations $T_g f \mapsto f(g^{-1}\cdot)$ and $T^g f \mapsto f(\cdot g)$ of functions on the group. A simple computation shows

$$\widehat{T_g f}(\pi) = \hat{f}(\pi)\pi^*(g) \quad \text{and} \quad \widehat{T^g f}(\pi) = \pi(g)\hat{f}(\pi).$$

They are direct consequences of the definition of the Fourier transform.

The Laplace-Beltrami operator $\Delta_{\mathcal{G}}$ of an invariant metric on the group \mathcal{G} is bi-invariant, i.e. commutes with all T_g and T^g . Therefore, all its eigenspaces are bi-invariant subspaces of $L^2(\mathcal{G})$. As H_π are minimal bi-invariant subspaces, each of them has to be eigenspace of $\Delta_{\mathcal{G}}$ with corresponding eigenvalue $-\lambda_\pi^2$. Hence, we obtain

$$\Delta_{\mathcal{G}} f = - \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \lambda_\pi^2 \text{trace}(\pi(g)\hat{f}(\pi)).$$

4. PROBLEM 5: RADON TRANSFORM ON COMPACT GROUPS

4.1. Radon transform.

Definition 1. *Let \mathcal{H} be a subgroup of the compact Lie group \mathcal{G} . The Radon transform \mathcal{R} of an integrable function f on \mathcal{G} is defined by*

$$(6) \quad \mathcal{R}f(x, y) = \int_{\mathcal{H}} f(xhy^{-1}) dh, \quad x, y \in \mathcal{G},$$

where dh denotes the normalized Haar measure on \mathcal{H} .

The range of $\mathcal{R}f$ should be contained in $\mathcal{G} \times \mathcal{G}$.

Lemma 2 ([2]). *The Radon transform (6) is invariant under right shifts of x and y , hence the range is a subset of $\mathcal{G}/\mathcal{H} \times \mathcal{G}/\mathcal{H}$.*

Proof. First, we take the Fourier transform of $\mathcal{R}f$ with respect to the x and let y be fixed and regard $\mathcal{R}f(x, y)$ as a function of $x \in \mathcal{G}$ only then

$$\widehat{\mathcal{R}f(\cdot, y)}(\pi) = \pi_{\mathcal{H}}\pi^*(y)\hat{f}(\pi), \quad \pi \in \hat{\mathcal{G}}.$$

It is easily seen that $\mathcal{R}f(x, y)$ is invariant under the projection $\mathbb{P}_{\mathcal{H}}$ and we obtain

$$\mathcal{R}f(x \cdot h, y) = \mathcal{R}f(x, y) \quad \forall h \in \mathcal{H}.$$

If we look at the Radon transform as a function in y while the first argument x is fixed, we find

$$\begin{aligned} \mathbb{P}_{\mathcal{H}}(\mathcal{R}f)(x, y) &= \int_{\mathcal{H}} \mathcal{R}f(x, yh) dh = \int_{\mathcal{H}} \sum_{\pi \in \hat{G}} d_\pi \text{trace}(\hat{f}(\pi)\pi(x)) \pi_{\mathcal{H}}\pi(h^{-1}y^{-1}) dh \\ &= \sum_{\pi \in \hat{G}} d_\pi \text{trace}(\hat{f}(\pi)\pi(x)) \pi_{\mathcal{H}}\pi^*(y) = (\mathcal{R})f(x, y). \end{aligned}$$

Consequently, $\mathcal{R}f(x, y)$ is constant over fibers of the form $y\mathcal{H}$ and

$$\widehat{\mathcal{R}f(x, \cdot)}(\pi) = \pi_{\mathcal{H}}\pi^*(x)\hat{f}(\pi), \quad \pi \in \hat{\mathcal{G}}.$$

□

We have just proven that this Radon transform act as a projection from $\mathcal{G} \rightarrow \mathcal{G}/\mathcal{H}$. To fix the mapping properties we need function spaces. We start with $L^2(\mathcal{G}/\mathcal{H} \times \mathcal{G}/\mathcal{H})$ and get the following theorem.

Theorem 3 ([2]). *Let \mathcal{H} be a subgroup of \mathcal{G} which determines the Radon transform on \mathcal{G} and let $\hat{\mathcal{G}}_1 \subset \hat{G}$ be the set of irreducible representations with respect to \mathcal{H} . Then for $f \in C^\infty(\mathcal{G})$ we have*

$$\|\mathcal{R}f\|_{L^2(\mathcal{G}/\mathcal{H} \times \mathcal{G}/\mathcal{H})}^2 = \sum_{\pi \in \hat{\mathcal{G}}_1} \text{rank}(\pi_{\mathcal{H}}) \|\hat{f}\|_{HS}^2.$$

Proof. We expand $\mathcal{R}f(x, y)$ for fixed y into a series with respect to x and apply Parseval's theorem

$$\begin{aligned} \|\mathcal{R}f\|_{L^2(\mathcal{G}/\mathcal{H} \times \mathcal{G}/\mathcal{H})}^2 &= \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \int_{\mathcal{G}} \|\pi_{\mathcal{H}}\pi^*(y)\hat{f}(\pi)\|_{HS}^2 dy \\ &= \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \int_{\mathcal{G}} \text{trace}(\hat{f}^*(\pi)\pi(y)\pi_{\mathcal{H}}\pi^*(y)\hat{f}(\pi)) dy \\ &= \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \text{trace}(\hat{f}^*(\pi) \left(\int_G \pi(y)\pi_{\mathcal{H}}\pi^*(y) dy \right) \hat{f}(\pi)) \\ &= \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \text{trace}(\hat{f}^*(\pi) \left(\sum_{k=1}^{\text{rank } \pi_{\mathcal{H}}} \int_G \pi_{ik}(y) \overline{\pi_{kj}(y)} dy \right)_{i,j=1}^{d_\pi} \hat{f}(\pi)) \\ &= \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \text{trace}(\hat{f}^*(\pi) \frac{\text{rank } \pi_{\mathcal{H}}}{d_\pi} Id \hat{f}(\pi)) \\ &= \sum_{\pi \in \hat{\mathcal{G}}} \text{rank } \pi_{\mathcal{H}} \text{trace}(\hat{f}^*(\pi)\hat{f}(\pi)) \\ &= \sum_{\pi \in \hat{\mathcal{G}}_1} \text{rank}(\pi_{\mathcal{H}}) \|\hat{f}\|_{HS}^2. \end{aligned}$$

□

From that we can conclude that the Radon transform is an isometry between $L(\mathcal{G})$ and some space on $\mathcal{G}/\mathcal{H} \times \mathcal{G}/\mathcal{H}$ but that doesn't say what is the right space. For that we start from the other side, i.e. we start with the L^2 -norm of f .

4.2. Mapping properties. We will need some help from harmonic analysis. The goal here is to find a Hilbert space structure such that the Radon transform is an isometry, which means that

$$\begin{aligned} \|f\|_{L^2(\mathcal{G})}^2 &= \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \|\hat{f}(\pi)\|_{HS}^2 = \sum_{\pi \in \hat{\mathcal{G}}} d_\pi \|\hat{f}(\pi)\|_{L^2(\mathcal{G}/\mathcal{H} \times \mathcal{G}/\mathcal{H})}^2 \\ &= \| \mathcal{R}f \|_{L^2(\mathcal{G}/\mathcal{H} \times \mathcal{G}/\mathcal{H})}^2 \end{aligned}$$

Suppose that the compact Lie group \mathcal{G} acts transitively on a compact Riemannian manifold \mathcal{M} as a group of isometries. Then if we set

$$l(g)f(x) = f(g^{-1}x), \quad g \in \mathcal{G}, \quad x \in \mathcal{M},$$

we have a unitary representation of \mathcal{G} on $L^2(\mathcal{M})$. Now if Δ is the Laplace operator, we have

$$l(g)\Delta = \Delta l(g), \quad g \in \mathcal{G}.$$

Thus the eigenspaces

$$V_\lambda = \{u \in C^\infty(\mathcal{M}) : \Delta u = -\lambda^2 u\}$$

of the Laplace operator, we have

$$l(g) : V_\lambda \rightarrow V_\lambda,$$

for each eigenvalue $-\lambda^2$.

Lemma 4 ([26], page 120). *If \mathcal{M} is a compact rank one symmetric space, then \mathcal{G} acts irreducibly on each eigenspace V_λ of Δ on \mathcal{M} .*

Examples of such compact rank one symmetric spaces following [26] are

$$\begin{aligned} \mathcal{G} &= SO(n+1), \quad \mathcal{M} = S^n, \\ \mathcal{G} &= SU(n+1), \quad \mathcal{M} = \mathbb{C}P^n (\text{complex projective plane}). \end{aligned}$$

Definition 2. *A representation $l(g)$ is called a representation of class-1 relative to \mathcal{H} if in its space there are nonzero vectors invariant relative to \mathcal{H} and the restriction of $l(g)$ to \mathcal{H} is unitary.*

Lemma 5 ([26], page 121, 122). *If $\mathcal{M} = \mathcal{G}/\mathcal{H}$ is a rank one symmetric space, with \mathcal{H} connected, then $L^2(\mathcal{M})$ contains each class-1 representation, exactly once, as an eigenspace of Δ .*

Therefore we will try to build up a norm from the eigenspaces of Δ which span some subspace of $L^2(\mathcal{M})$ and consider the case $\mathcal{G} = SO(n+1)$, $\mathcal{H} = SO(n)$ in more detail.

4.3. The case $\mathcal{G} = SO(n+1)$ and $\mathcal{H} = SO(n)$. The following result is well-known.

Lemma 6. *The space*

$$L^2(S^{n-1}) = \bigoplus_k \mathcal{H}_k,$$

where \mathcal{H}_k is the space of harmonic polynomials, homogeneous of degree k , $k \in \mathbb{N}_0$.

Both previously mentioned lemmas together are only fulfilled for S^2 , in this case we have

Lemma 7 ([26], page 140). *The decomposition*

$$L^2(S^2) = \bigoplus_k V_k$$

contains each irreducible unitary representation of $SO(3)$, exactly once.

But also for higher dimensional spheres we have some nice results. We start with the orthonormal system of spherical harmonics $\mathcal{Y}_k^i \in C^\infty(S^n)$, $k \in \mathbb{N}_0$, $i = 1, \dots, d_k(n)$ normalized with respect to the Lebesgue measure on S^n . Obviously $\mathcal{H}_k = \text{span} \{\mathcal{Y}_k^i\}_{i=1}^{d_k(n)}$. Then the Wigner polynomials on $SO(n+1)$ $\mathcal{T}_k^{ij}(g)$, $g \in SO(n+1)$ are given by

$$\mathcal{T}_k^{ij}(g) = \int_{S^n} \mathcal{Y}_k^i(g^{-1}x) \overline{\mathcal{Y}_k^j(x)} dx$$

and due to orthogonality of the spherical harmonics

$$\mathcal{Y}_k^i(g^{-1}x) = \sum_{j=1}^{d_k(n)} \mathcal{T}_k^{ij}(g) \mathcal{Y}_k^j(x).$$

From these properties and the orthonormality of the spherical harmonics it is easy to see that the Wigner polynomials build an orthonormal system in $L^2(SO(n+1))$. Unfortunately, Wigner polynomials do not give all irreducible unitary representations of $SO(n+1)$ if $n \geq 2$. (Compare with Lemma 7.)

Definition 3. *Let \mathcal{L} be a linear space of functions $f(x)$, $f \in \mathcal{G}$, $x \in \mathcal{M}$. If in the space \mathcal{L} of any representation of class-1 relative \mathcal{H} there is only one normalized invariant vector, then \mathcal{H} is called a massive subgroup.*

Lemma 8 ([27], Chapter IX.2). *$SO(n)$ is a massive subgroup of $SO(n+1)$. Furthermore, the family \mathcal{T}_k , $k \in \mathbb{N}_0$, gives up to equivalence all class-1 representations of $SO(n+1)$ with respect to $SO(n)$.*

For the following let x_0 be the base point of $SO(n+1)/SO(n) \sim S^n$ (x_0 is usually chosen to be the "north pole".) In this case the set of zonal spherical harmonics is one-dimensional and spanned by the Gegenbauer polynomials $\mathcal{C}_k^{(n-1)/2}(x_0^T x)$. We recall some helpful and well known results.

Lemma 9 (Addition theorem). *For all $x, y \in S^n$, $k \in \mathbb{N}_0$ and $i = 1, \dots, d_k(n)$*

$$\frac{\mathcal{C}_k^{(n-1)/2}(x^T y)}{\mathcal{C}_k^{(n-1)/2}(1)} = \frac{|S^n|}{d_k(n)} \sum_{i=1}^{d_k(n)} \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^i(y)}.$$

Lemma 10 (Zonal averaging).

$$\int_{SO(n)} \mathcal{Y}_k^i(gx) dg = \frac{\mathcal{Y}_k^i(x_0)}{\mathcal{C}_k^{(n-1)/2}(1)} \mathcal{C}_k^{(n-1)/2}(x_0^T x).$$

Lemma 11 (Funk-Hecke formula). *Let $f : [-1, 1] \rightarrow \mathcal{C}$ be continuous. Then for all $i = 1, \dots, d_k(n)$*

$$\int_{S^n} f(x^T y) \mathcal{Y}_k^i(x) dx = \mathcal{Y}_k^i(y) \frac{|S^{n-1}|}{\mathcal{C}_k^{(n-1)/2}(1)} \int_{-1}^1 f(t) \mathcal{C}_k^{(n-1)/2}(t) (1-t^2)^{n/2-1} dt.$$

We look for all irreducible representations of $SO(n+1)$ which do not have vanishing coefficients under the projection $\mathbb{P}_{SO(n)}$. These are the class-1 representations of $SO(n+1)$ with respect to $SO(n)$ and the projections are given by

$$\begin{aligned} \mathbb{P}_{S^n} \mathcal{T}_k^{ij} &= \int_{SO(n)} \mathcal{T}_k^{ij}(g) dg = \int_{S^n} \int_{SO(n)} \mathcal{Y}_k^i(g^{-1}x) dg \mathcal{Y}_k^j(x) dx \\ &= \frac{\mathcal{Y}_k^i(x_0)}{\mathcal{C}_k^{(n-1)/2}} \int_{S^n} \mathcal{C}_k^{(n-1)/2}(x_0^T x) \mathcal{Y}_k^j(x) dx \\ &= \frac{\mathcal{Y}_k^i(x_0) \mathcal{Y}_k^j(x_0)}{(\mathcal{C}_k^{(n-1)/2}(1))^2} |S^n| \int_{-1}^1 (\mathcal{C}_k^{(n-1)/2}(t))^2 (1-t^2)^{n/2-1} dt \\ &= \frac{|S^n|}{d_k(n)} \mathcal{Y}_k^i(x_0) \mathcal{Y}_k^j(x_0), \end{aligned}$$

due to the Funk-Hecke formula and the normalization of Gegenbauer polynomials. We assume that the basis of spherical harmonics $\mathcal{Y}_k^i(x)$ is chosen such that $\mathcal{Y}_k^1(x_0) = \sqrt{\frac{d_k(n)}{|S^n|}}$ and $\mathcal{Y}_k^i(x_0) = 0$ for all $i > 1$, then

$$\sqrt{\frac{|S^n|}{d_k(n)}} \mathcal{Y}_k^i(x) = (\mathbb{P}_{S^n} \mathcal{T}_k^{i1})(x) = \int_{SO(n)} \mathcal{T}_k^{i1}(gh) dh = \mathcal{T}_k^{i1}(g), \quad x = gx_0.$$

Now we calculate the Radon transform from the span $(\mathcal{T}_k)_{k \in \mathbb{N}_0}$ into $S^n \times S^n$. Let be

$$f(g) = \sum_{k=0}^{\infty} \sum_{i,j=1}^{d_k(n)} \hat{f}(k)_{ij} \mathcal{T}_k^{ij}$$

then

$$\begin{aligned} \mathcal{R}f(x, y) &= \sum_{k=0}^{\infty} d_k(n) \text{trace}(\hat{f}(k) \mathcal{T}_k(x) \pi_{SO(n)} \mathcal{T}_k^*(y)) \\ &= \sum_{k=0}^{\infty} d_k(n) \sum_{i,j=1}^{d_k(n)} \hat{f}(k)_{ij} \mathcal{T}_k^{i1}(x) \overline{\mathcal{T}_k^{1j}(y)} \\ &= \sum_{k=0}^{\infty} \frac{|S^n|}{d_k(n)} d_k(n) \sum_{i,j=1}^{d_k(n)} \hat{f}(k)_{ij} \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)} \\ &= |S^n| \sum_{k=0}^{\infty} \sum_{i,j=1}^{d_k(n)} \hat{f}(k)_{ij} \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)} \end{aligned}$$

From the last equation it is easily seen that

$$(7) \quad \Delta_x \mathcal{R} = \Delta_y \mathcal{R}.$$

Which also means that the image is a subspace of $L^2(S^n \times S^n)$ rather than the whole space. It also follows that for the Fourier coefficients of $g = \mathcal{R}f$ we have

$$(8) \quad \hat{g}(k)_{ij} = |S^n| \hat{f}(k)_{ij} \iff \hat{f}(k)_{ij} = \frac{1}{|S^n|} \hat{g}(k)_{ij}.$$

5. PROBLEM 2: RADON TRANSFORM ON $SO(3)$

Problem 3 can be derived from Problem 5 by choosing $\mathcal{G} = SO(3)$, $\mathcal{H} = SO(2)$ and thus $\mathcal{G}/\mathcal{H} = SO(3)/SO(2) = S^2$. In this special situation all irreducible representations are equivalent to an irreducible component of the left regular representation

$$T(g) : f(x) \mapsto f(g^{-1} \cdot x),$$

where \cdot denotes the canonical action of $SO(3)$ on S^2 . The T invariant subspaces of $L^2(S^2)$ are $\mathcal{H}_k = \{\mathcal{Y}_k^i, i = 1, \dots, 2k+1\}$, which are spanned by all spherical harmonics of degree k . It is well known that the eigenvalues of the Laplacian on $SO(3)$ and on S^2 corresponding to polynomials of degree k is $-k(k+1)$, i.e.

$$\Delta_{SO(3)} \mathcal{T}_k^{ij} = -k(k+1) \mathcal{T}_k^{ij} \quad \text{and} \quad \Delta_{S^2} \mathcal{Y}_k^i = -k(k+1) \mathcal{Y}_k^i.$$

We will use that to define an appropriate norm for the Radon transform from $L^2(SO(3))$ onto an subspace of $L^2(S^2 \times S^2)$. Starting with the dimension of the representations space $d_\pi = 2k+1$ and $-\lambda_k^2 = -k(k+1)$ we get $d_k = \sqrt{1+4\lambda_k^2}$ and $\sqrt{d_k} = \sqrt[4]{2(\lambda_k^2 + \lambda_k^2 + 1)}$. Using (8) and the fact that Δ is equal to $-k(k+1)$ on the eigenspace \mathcal{H}_k we obtain

$$\|f\|_{L^2(SO(3))}^2 = \sum_{k=1}^{\infty} (2k+1) \|\hat{f}(k)\|_{HS}^2 =$$

$$\sum_{k=1}^{\infty} (2k+1) \|(4\pi)^{-1} \hat{f}(k)\|_{L^2(S^2 \times S^2)}^2 = \|(4\pi)^{-1} (-2(\Delta_1 + \Delta_2) + 1)^{1/4} \mathcal{R}f\|_{L^2(S^2 \times S^2)}^2,$$

where $\Delta_1 + \Delta_2$ is a Laplace operator on $S^2 \times S^2$. Thus we define the following norm for $u \in C^\infty(S^2 \times S^2)$

$$\|u\|^2 = ((-2\Delta_{S^2 \times S^2} + 1)^{1/2} u, u)_{L^2(S^2 \times S^2)},$$

where $\Delta_{S^2 \times S^2} = \Delta_1 + \Delta_2$.

Because we have an isometry (up to a constant) the inverse operator is given by the adjoint of \mathcal{R} . To calculate the adjoint operator we express the Radon transform in another way. Going back to our problem in crystallography we first state that the great circle $C_{x,y}$ is given by

$$C_{x,y} = x' SO(2)(y')^{-1} := \{x' h(y')^{-1}, h \in SO(2)\}, \quad x', y' \in SO(3),$$

and $x' \cdot x_0 = x$, $y' \cdot x_0 = y$ with $SO(2)$ being the stabilizer of $x_0 \in S^2$. Hence,

$$\begin{aligned}\mathcal{R}f(x, y) &= \int_{SO(2)} f(xhy^{-1}) dh = 4\pi \int_{C_{x,y}} f(g) dg \\ &= 4\pi \int_{SO(3)} f(g) \delta_y(g^{-1} \cdot x) dg, \quad f \in L^2(SO(3)),\end{aligned}$$

where $C_{x,y} = \{g \in SO(3) : g \cdot x = y\}$ is a great circle in $SO(3)$. To calculate the adjoint operator we will use the last representation of \mathcal{R} . We have

$$\begin{aligned}(\mathcal{R}^*u, f)_{L^2(SO(3))} &= ((-2\Delta_{S^2 \times S^2} + 1)^{1/2}u, \mathcal{R}f)_{L^2(S^2 \times S^2)} = \\ &= (4\pi) \int_{S^2 \times S^2} (-2\Delta_{S^2 \times S^2} + 1)u(x, y) \int_{SO(3)} f(g) \delta_y(g^{-1} \cdot x) dg dx dy = \\ &= (4\pi) \int_{SO(3)} \int_{S^2} (-2\Delta_{S^2 \times S^2} + 1)^{1/2}u(g \cdot y, y) dy f(g) dg,\end{aligned}$$

i.e. the L^2 -adjoint operator is given by

$$(9) \quad \mathcal{R}^*u = (4\pi) \int_{S^2} (-2\Delta_{S^2 \times S^2} + 1)^{1/2}u(g \cdot y, y) dy.$$

Definition 4 (Sobolev spaces on $S^2 \times S^2$). *The Sobolev space $H_t(S^2 \times S^2)$, $t \in \mathbb{R}$, is defined as the domain of the operator $(1 - 2\Delta_{S^2 \times S^2})^{\frac{t}{2}}$ with graph norm*

$$\|f\|_t = \|(1 - 2\Delta_{S^2 \times S^2})^{\frac{t}{2}}f\|_{L^2(S^2 \times S^2)},$$

and the Sobolev space $H_t^\Delta(S^2 \times S^2)$, $t \in \mathbb{R}$, is defined as the subspace of all functions $f \in H_t(S^2 \times S^2)$ such $\Delta_1 f = \Delta_2 f$.

and

Definition 5 (Sobolev spaces on $SO(3)$). *The Sobolev space $H_t(SO(3))$, $t \in \mathbb{R}$, is defined as the domain of the operator $(1 - 4\Delta_{SO(3)})^{\frac{t}{2}}$ with graph norm*

$$\|f\|_t = \|(1 - 4\Delta_{SO(3)})^{\frac{t}{2}}f\|_{L^2(SO(3))}, \quad f \in L^2(SO(3)).$$

Then:

Theorem 12. *For any $t \geq 0$ the Radon transform on $SO(3)$ is an invertible mapping*

$$(10) \quad \mathcal{R} : H_t(SO(3)) \rightarrow H_{t+\frac{1}{2}}^\Delta(S^2 \times S^2).$$

and

$$(11) \quad f(g) = \int_{S^2} (-2\Delta + 1)^{\frac{1}{2}}(\mathcal{R}f)(gy, y) dy = \frac{1}{4\pi}(\mathcal{R}^*\mathcal{R}f)(g).$$

Proof. For the mapping properties it is sufficient to consider case $t = 0$. Because the Radon transform is only an isometry up to 4π , we obtain (11). \square

Since

$$\mathcal{R}(\mathcal{T}^k)(x, y) = \mathcal{T}^k(x) \pi_{SO(2)} \left(\mathcal{T}^k(y) \right)^*$$

we have

$$\mathcal{R}\mathcal{T}_{ij}^k(x, y) = \mathcal{T}_{i1}^k(x) \overline{\mathcal{T}_{j1}^k(y)} = \frac{4\pi}{2k+1} \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)}.$$

Theorem 13 (Reconstruction formula). *Let*

$$G(x, y) = \mathcal{R}f(x, y) = \sum_{k=0}^{\infty} \sum_{i,j=1}^{2k+1} \widehat{G}(k)_{ij} \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)} \in H_{\frac{1}{2}+t}^{\Delta}(S^2 \times S^2), \quad t \geq 0,$$

be the result of a Radon transform. Then the pre-image $f \in H_t(SO(3))$, $t \geq 0$, is given by

$$\begin{aligned} f &= \sum_{k=0}^{\infty} \sum_{i,j=1}^{2k+1} \frac{(2k+1)}{4\pi} \widehat{G}(k)_{ij} \mathcal{T}_{ij}^k = \sum_{k=0}^{\infty} \sum_{i,j=1}^{2k+1} (2k+1) \widehat{f}(k)_{ij} \mathcal{T}_{ij}^k \\ &= \sum_{k=0}^{\infty} (2k+1) \text{trace}(\widehat{f}(k) \mathcal{T}^k). \end{aligned}$$

6. THE GROUP $SO(3)$ AND THE SPHERE S^3

Since S^3 is a double cover of $SO(3)$ every function f on $SO(3)$ can be identified with an even function on S^3 . After such identification the crystallographic Radon transform on $SO(3)$ becomes the Funk transform on S^3 . In this section we show how some known results for Funk transform can be interpreted in crystallographic terms.

Let \mathcal{C} denote the set of all 1-dimensional totally geodesic submanifolds $C \subset S^3$. Each $C \in \mathcal{C}$ is a 1-sphere, i.e. a circle with centre \mathcal{O} . Each circle is characterized by a unique pair of unit vectors $(h, r) \in S^2 \times S^2$.

Thus, the pole density function can be rewritten as

$$Pf(h, r) = \frac{1}{8\pi} \int_{C \cup C^\perp} f(q) d\omega_1(q),$$

where the circle $C \subset S^3$ represents all rotations mapping $h \in S^2$ on $r \in S^2$ and where $C^\perp(q_1, q_2)$ is the orthogonal circle representing all rotations mapping $-h$ on r , and where ω_1 denotes the usual one-dimensional circular Riemann measure.

Following Helgason (see [12], [13], [14]), we introduce the next definition.

Definition 6. *For a continuous function f defined on S^3 its 1-dimensional spherical (totally geodesic) Radon transform $\mathcal{R}f$ is a function, which is defined on any 1-dimensional totally geodesic submanifold $C \subset S^3$ by the following formula*

$$(\mathcal{R}f)(C) = \frac{1}{2\pi} \int_C f(q) d\omega_1(q) = \int_C f(q) dm(q),$$

with the normalized measure $m = \frac{1}{2\pi} \omega_1$.

The Radon transform of f may be represented as the convolution of f with the indicator function of the great circle C . It associates with the function f its mean values over great circles $C \in \mathcal{C}$. Since each great circle is uniquely characterized by a pair $(h, r) \in S^2 \times S^2$ (see [21]) and its antipodally symmetric, we also use the notation $(\mathcal{R}f)(h, r) \equiv (\mathcal{R}f)(-h, -r)$ whenever it is more instructive.

It should be noted that no distinction has been made whether f refers to $SO(3)$ or S^3 , even though the form of f depends on the representation of g ; in particular, with respect to S^3 only even functions f could be orientation probability density functions as $q \in S^3$ and $-q$ represent the same orientation.

Thus, one has

$$(12) \quad Pf(h, r) = \frac{1}{4} \left((\mathcal{R}f)(C_{h,r}) + (\mathcal{R}f)(C_{-h,r}) \right),$$

where $P(h, r)$ is again the crystallographic X-ray transform.

The following definition of the generalized 1-dimensional spherical Radon transform and the respective dual can be found in [13], [14].

Definition 7. *The generalized 1-dimensional spherical Radon transform of a real function $f : S^3 \mapsto \mathbb{R}_1$ is defined as*

$$(\mathcal{R}^{(\rho)}f)(C) = \frac{1}{4\pi^2 \sin \rho} \int_{d(q,C)=\rho} f(q) dq.$$

The next definition was introduced in [1], and [9], p. 64.

Definition 8. *The spherically generalized translation of a real function $F \in C(S^2)$ or $F \in L^p(S^2)$, $1 \leq p < \infty$, is defined as*

$$(\mathcal{T}_2^{(\rho)}F)(r) = \frac{1}{2\pi \sqrt{1 - \cos^2 \rho}} \int_{r \cdot r' = \cos \rho} F(r') dr'.$$

where $2\pi \sqrt{1 - \cos^2 \rho}$ is the length of the circle $c(r; \rho)$ centered at r with radius $\cos \rho$.

To describe connection between Radon transform and other operators it is useful to introduce the angle density function

$$((\mathcal{A}f)(h, r; \rho) = R^{(\rho/2)}f)(C_{h,r}).$$

Note, that $(\mathcal{A}f)(h, r; \rho)$ has been introduced in [6], p. 44 and [7], p. 74, but with a false normalization.

The following statement holds.

Proposition 3. *The generalized 1-dimensional spherical Radon transform is equal to the translated spherical Radon transform and it can be identified with the angle density function*

$$(13) \quad \left(\mathcal{T}_2^{(\rho)}[\mathcal{R}f] \right)(h, r) = (\mathcal{R}^{(\rho/2)}f)(C_{h,r}) = (\mathcal{A}f)(h, r; \rho)$$

The proof can be found in [4].

The following properties should be noted

$$(14) \quad \begin{aligned} (\mathcal{A}f)(h, r; 0) &= (\mathcal{R}f)(h, r), \\ (\mathcal{A}f)(h, r; \pi) &= (\mathcal{R}f)(h, -r). \end{aligned}$$

According to its definition the quantity $(\mathcal{A}f)(h, r; \pi)$ it is the mean value of the spherical pole probability density function over any small circle centered at r . Thus, it is the probability density that the crystallographic direction h statistically encloses the angle ρ , $0 \leq \rho \leq \pi$, with the specimen direction r given the orientation probability density function f . Its central role for the inverse Radon transform was recognized in [18] [19].

The next two definitions were given by Helgason in [13], [14].

Definition 9. *The dual 1-dimensional spherical Radon transform of a real continuous function $\varphi : \mathcal{C} \mapsto \mathbb{R}_1$ is defined as*

$$(\tilde{\mathcal{R}}\varphi)(q) = \int_{C \ni q} \varphi(C) d\mu(C),$$

where μ denotes the unique measure on the compact space $C \in \mathcal{C} : q \in C$, invariant under all rotations around q , and having total measure 1.

Thus $(\tilde{\mathcal{R}}\varphi)(q)$ is the mean value of φ over the set of circles $C \in \mathcal{C}$ passing through q .

Definition 10. *The dual generalized 1-dimensional spherical Radon transform of a real continuous function $\varphi : \mathcal{C} \mapsto \mathbb{R}_1$ is defined as*

$$(\tilde{\mathcal{R}}^{(\rho)}\varphi)(q) = \int_{\{C \in \mathcal{C} : d(q, C) = \rho\}} \varphi(C) d\tilde{\mu}(C).$$

With the normalized measure $\tilde{\mu} = A^{-1}(\rho)d\mu$, $A(\rho) = 4\pi \sin^2 \rho$, it is the mean value of φ over the set of all circles $C \in \mathcal{C}$ with distance ρ from q .

One has that $(\tilde{\mathcal{R}}^{(\rho)}(\mathcal{R}f))(q)$ is the mean value of $(\mathcal{R}f)$ over the set of all circles $C \in \mathcal{C}$ with distance ρ from q , i.e. tangential to the sphere $s(q; \rho)$. More specifically, with the usual two-dimensional spherical Riemann measure ω_2 ,

$$\begin{aligned} (\tilde{\mathcal{R}}^{(\rho)}(\mathcal{R}f))(q) &= \int_{d(q, C) = \rho} (\mathcal{R}f)(C_{h,r}) d\tilde{\mu}(C_{h,r}) \\ &= \frac{1}{4\pi \sin(2\rho)} \int_{S^2} \int_{c(gh; 2\rho)} (\mathcal{R}f)(C_{h,r}) dr d\omega_2(h) \\ (15) \quad &= \frac{1}{2} \int_{S^2} (\mathcal{A}f)(h, gh; 2\rho) d\omega_2(h) \\ &= \frac{1}{2} \int_{S^2} (\mathcal{R}^{(\rho)}f)(C_{h,gh}) d\omega_2(h) \\ (16) \quad &= (\tilde{\mathcal{R}}(\mathcal{R}^{(\rho)}f))(q), \end{aligned}$$

which is instrumental for the inversion of the spherical Radon transforms.

Now, we use the inversion formula of S. Helgason [14], which was obtained for the general case two-point homogeneous spaces. For two dimensional sphere the totally geodesic Radon transform is also known as Funk transform. We start with the inversion formula and derive a connection to the angle density function $\mathcal{A}f$. The inversion formula reads as

$$f(q) = \frac{1}{2\pi} \left[\frac{d}{du} \int_0^u \left(\tilde{\mathcal{R}}^{(\arccos v)}(\mathcal{R}f) \right)(q) \frac{v}{\sqrt{u^2 - v^2}} dv \right]_{u=1}.$$

Moreover, one can use angle density function $\mathcal{A}f$ to deduce Matthies' inversion formula, which was obtained in [19]. One starts with (15) to obtain

$$\begin{aligned} f(q) &= \frac{1}{4\pi} \left[\frac{d}{du} \int_0^u \int_{S^2} (\mathcal{A}f)(h, gh; 2 \arccos v) d\omega_2(h) \frac{v}{\sqrt{u^2 - v^2}} dv \right]_{u=1} = \\ &= \frac{1}{4\pi} \left(\int_{S^2} (\mathcal{A}f)(h, gh; \pi) d\omega_2(h) \right. \\ &\quad \left. + \int_0^s \int_{S^2} \frac{d}{ds} (\mathcal{A}f)(h, gh; 2 \arccos \sqrt{s-w}) dh \frac{1}{\sqrt{w}} dw \right) \Big|_{s=1}. \end{aligned}$$

Using the formula

$$\frac{d}{ds} (\mathcal{A}f) = -\frac{d}{dw} (\mathcal{A}f)$$

and taking into account

$$(\mathcal{A}f)(h, gh; \pi) = (\mathcal{R}f)(h, gh)$$

(cf. Eq. (14)), one obtains for $2w = 1 - \cos \theta$ and $s = 1$ the desired inversion formula:

$$\begin{aligned} f(q) &= \frac{1}{4\pi} \left(\int_{S^2} (\mathcal{R}f)(h, gh) d\omega_2(h) \right. \\ &\quad \left. + 2 \int_0^\pi \int_{S^2} \frac{d}{d \cos \theta} ((\mathcal{A}f)(h, gh; \theta)) d\omega_2(h) \cos \frac{\theta}{2} d\theta \right). \end{aligned}$$

The practical importance of this formula is that $\mathcal{A}f$ is easily experimentally accessible and might yield an improved inversion compared to inverting just pole intensities. This formula was already obtained in [3] and is equivalent to the formula in [20] which was given without any proof.

7. PROBLEM 1: ON INVERSION OF CRYSTALLOGRAPHIC X -RAY TRANSFORM

Unfortunately, neither with the Radon transform \mathcal{R} over $SO(3)$ nor with the Radon transform \mathcal{R} over S^3 we are solving the crystallographic problem. The point is that since

$$\mathcal{Y}_k^i(-x) = (-1)^k \mathcal{Y}_k^i(x),$$

one has for $G(x, y) = \mathcal{R}f(x, y)$:

$$\begin{aligned}
Pf(x, y) &= \frac{1}{2} (\mathcal{R}f(x, y) + \mathcal{R}f(-x, y)) = \frac{1}{2} (G(x, y) + G(-x, y)) \\
&= \frac{1}{2} \left(\sum_{k=0}^{\infty} \sum_{i,j=1}^{2k+1} \hat{G}(k)_{ij} \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)} + \sum_{k=0}^{\infty} \sum_{i,j=1}^{2k+1} \hat{G}(k)_{ij} \mathcal{Y}_k^i(-x) \overline{\mathcal{Y}_k^j(y)} \right) \\
&= \frac{1}{2} \left(\sum_{k=0}^{\infty} \sum_{i,j=1}^{2k+1} \hat{G}(k)_{ij} \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)} + \sum_{k=0}^{\infty} (-1)^k \sum_{i,j=1}^{2k+1} \hat{G}(k)_{ij} \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)} \right) \\
&= \sum_{l=0}^{\infty} \sum_{i,j=1}^{4l+1} \hat{G}(2l)_{ij} \mathcal{Y}_{2l}^i(x) \overline{\mathcal{Y}_{2l}^j(y)}.
\end{aligned}$$

In other words we lose half of the data needed for the reconstruction, because the experiment (which is measuring PDF Pf) only gives the even coefficients $\hat{G}(2l)_{ij}$.

Since odd Fourier coefficients $\hat{G}(2l+1)_{ij}$ of the function $G(x, y) = \mathcal{R}f(x, y)$ disappear one cannot reconstruct the function $f(g)$, $g \in SO(3)$, from $Pf(x, y)$. Note that we have two additional conditions stemming from the fact that f is a probability distribution function:

- (1) $f(g) \geq 0$, i.e. f is non-negative,
- (2) $\int_{SO(3)} f(g) dg = 1$.

The second condition is just a normalization, the first condition is less trivial.

We obviously can reconstruct the even part $f_e(g)$ from the even coefficients $\hat{G}(2l)_{ij}$. A legitimate question to ask is the following: Does there exist an odd part $f_o(g)$ such that $f(g) = f_e(g) + f_o(g) \geq 0$ and $f_o(g)$ is uniquely determined?

8. PROBLEM 4: EXACT RECONSTRUCTION OF BANDLIMITED FUNCTIONS ON $SO(3)$ FROM A FINITE NUMBER OF SAMPLES OF THEIR RADON TRANSFORM

It is clear that in practice one has to face situations described in Problems 3 and 4. Concerning Problem 3 we refer to [8] where approximate inverse was found using language of Gabor frames. A solution to the Problem 4 will be described in the present section.

Let $B((x, y), r)$ be a metric ball on $S^2 \times S^2$ whose center is (x, y) and radius is r .

As it explained in Appendix there exists a natural number $N_{S^2 \times S^2}$, such that for any sufficiently small $\rho > 0$ there exists a set of points $\{(x_\nu, y_\nu)\} \subset S^2 \times S^2$ such that:

- (1) the balls $B((x_\nu, y_\nu), \rho/4)$ are disjoint,
- (2) the balls $B((x_\nu, y_\nu), \rho/2)$ form a cover of $S^2 \times S^2$,

(3) the multiplicity of the cover by balls $B((x_\nu, y_\nu), \rho)$ is not greater than $N_{S^2 \times S^2}$.

Any set of points, which has properties (1)-(3) will be called a metric ρ -lattice.

For an $\omega > 0$ let us consider the space $\mathbf{E}_\omega(SO(3))$ of ω -bandlimited functions on $SO(3)$ i.e. the span of all Wigner functions T_{ij}^k with $k(k+1) \leq \omega$.

The goal of this section is to prove the following discrete reconstruction formula (18) for functions f in $\mathbf{E}_\omega(SO(3))$, which uses only a *finite* number of samples of $\mathcal{R}f$.

Theorem 14. (*Discrete Inversion Formula*)

There exists a $C > 0$ such that for any $\omega > 0$, if

$$\rho = C(\omega + 1)^{-1/2},$$

then for any ρ -lattice $\{(x_\nu, y_\nu)\}_{\nu=1}^{m_\omega}$ of $S^2 \times S^2$, there exist positive weights

$$\mu_\nu \asymp \omega^{-2},$$

such that for every function f in $\mathbf{E}_\omega(SO(3))$ the Fourier coefficients $c_{i,j}^k(\mathcal{R}f)$ of its Radon transform, i.e.

$$\mathcal{R}f(x, y) = \sum_{i,j,k} c_{i,j}^k(\mathcal{R}f) \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)}, \quad k(k+1) \leq \omega, \quad (x, y) \in S^2 \times S^2,$$

are given by the formulas

$$(17) \quad c_{i,j}^k(\mathcal{R}f) = \sum_{\nu=1}^{m_\omega} \mu_\nu (\mathcal{R}f)(x_\nu, y_\nu) \mathcal{Y}_k^i(x_\nu) \overline{\mathcal{Y}_k^j(y_\nu)}.$$

Moreover, the function itself can be reconstructed by means of the formula

$$(18) \quad f(g) = \sum_k \sum_{i,j}^{2k+1} \frac{(2k+1)}{4\pi} c_{i,j}^k(\mathcal{R}f) T_k^{i,j}(g), \quad g \in SO(3),$$

in which k runs over all natural numbers such that $k(k+1) \leq \omega$.

Proof. As the formulas

$$(19) \quad \Delta_{SO(3)} T_k^{ij} = -k(k+1) T_k^{ij}, \quad \Delta_{S^2} \mathcal{Y}_k^i = -k(k+1) \mathcal{Y}_k^i.$$

and

$$(20) \quad \mathcal{R}T_k^{ij}(x, y) = \frac{4\pi}{2k+1} \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)}$$

show the Radon transform of a function $f \in \mathbf{E}_\omega(SO(3))$ is ω -bandlimited on $S^2 \times S^2$ in the sense that its Fourier expansion involves only functions $\mathcal{Y}_k^i \overline{\mathcal{Y}_k^j}$ which are eigenfunctions of $\Delta_{S^2 \times S^2}$ with eigenvalue $-k(k+1)$. Let $\mathcal{E}_\omega(S^2 \times S^2)$ be the span of $\mathcal{Y}_k^i(\xi) \overline{\mathcal{Y}_k^j(\eta)}$. Thus

$$\mathcal{R} : \mathbf{E}_\omega(SO(3)) \rightarrow \mathcal{E}_\omega(S^2 \times S^2).$$

Let $\{(x_1, y_1), \dots, (x_m, y_m)\}$ be a set of pairs of points in $SO(3)$ and $\mathcal{M}_\nu = x_\nu SO(2)y_\nu^{-1}$ are corresponding submanifolds of $SO(3)$, $\nu = 1, \dots, m$.

For a function $f \in \mathbf{E}_\omega(SO(3))$ and a vector (of measurements) $v = (v_\nu)_1^m$ where

$$v_\nu = \int_{\mathcal{M}_\nu} f,$$

one has

$$\mathcal{R}f(x_\nu, y_\nu) = v_\nu.$$

We are going to find exact formulas for all Fourier coefficients of $\mathcal{R}f \in \mathcal{E}_\omega(S^2 \times S^2)$ in terms of a finite set of measurement. Since $SO(3)$ has dimension three then according to Theorem 16 (see Appendix) every product $(\mathcal{R}f) \mathcal{Y}_k^i \overline{\mathcal{Y}_k^j}$, where $k(k+1) \leq \omega$ belongs to $\mathcal{E}_\Omega(S^2 \times S^2)$, where $\Omega = 4 \times 6\omega = 24\omega$.

By the Theorem 15 (see Appendix) there exists a positive constant C , such that if $\rho = C(\omega + 1)^{-1/2}$, then for any ρ -lattice $\{(x_1, y_1), \dots, (x_{m_\omega}, y_{m_\omega})\}$ in $S^2 \times S^2$ there exist a set of positive weights

$$\mu_\nu \asymp \Omega^{-2}$$

such that

$$\begin{aligned} c_{i,j}^k(\mathcal{R}f) &= \int_{S^2 \times S^2} (\mathcal{R}f)(x, y) \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)} dx dy = \\ (21) \quad &\sum_{\nu=1}^N \mu_\nu (\mathcal{R}f)(x_\nu, y_\nu) \mathcal{Y}_k^i(x_\nu) \overline{\mathcal{Y}_k^j(y_\nu)}. \end{aligned}$$

Thus,

$$(\mathcal{R}f)(x, y) = \sum_{\nu} c_{i,j}^k(\mathcal{R}f) \mathcal{Y}_k^i(x) \overline{\mathcal{Y}_k^j(y)},$$

where

$$(22) \quad c_{i,j}^k(\mathcal{R}f) = \sum_{\nu=1}^N \mu_\nu (\mathcal{R}f)(x_\nu) \mathcal{Y}_k^i(x_\nu) \overline{\mathcal{Y}_k^j(x_\nu)}.$$

Now the reconstruction formula of Theorem 13 gives our result (18). \square

9. APPENDIX

We explain Theorems 15 and 16, which played key role in the proof of Theorem 14.

9.1. Positive cubature formulas on compact manifolds. We consider a compact connected Riemannian manifold \mathbf{M} . Let $B(\xi, r)$ be a metric ball on \mathbf{M} whose center is ξ and radius is r .

It was shown in [23], [24], that if \mathbf{M} is compact then there exists a natural number $N_{\mathbf{M}}$, such that for any sufficiently small $\rho > 0$ there exists a set of points $\{\xi_k\}$ such that:

- (1) the balls $B(\xi_k, \rho/4)$ are disjoint,
- (2) the balls $B(\xi_k, \rho/2)$ form a cover of \mathbf{M} ,
- (3) the multiplicity of the cover by balls $B(\xi_k, \rho)$ is not greater than $N_{\mathbf{M}}$.

Any set of points $M_\rho = \{\xi_k\}$ which has properties (1)-(3) will be called a metric ρ -lattice.

Let L be an elliptic second order differential operator on \mathbf{M} , which is self-adjoint and positive semi-definite in the space $L_2(\mathbf{M})$ constructed with respect to Riemannian measure. Such operator has a discrete spectrum $0 < \lambda_1 \leq \lambda_2 \leq \dots$ which goes to infinity and does not have accumulation points. Let $\{u_j\}$ be an orthonormal system of eigenvectors of L , which is complete in $L_2(\mathbf{M})$.

For a given $\omega > 0$ the notation $\mathbf{E}_\omega(L)$ will be used for the span of all eigenvectors u_j that correspond to eigenvalues not greater than ω .

Now we are going to prove existence of cubature formulas which are exact on $\mathbf{E}_\omega(L)$, and have positive coefficients of the "right" size.

The following exact cubature formula was established in [11], [25].

Theorem 15. *There exists a positive constant C , such that if*

$$\rho = C(\omega + 1)^{-1/2},$$

then for any ρ -lattice $M_\rho = \{\xi_k\}$, there exist strictly positive coefficients $\mu_{\xi_k} > 0$, $\xi_k \in M_\rho$, for which the following equality holds for all functions in $\mathbf{E}_\omega(L)$:

$$(23) \quad \int_{\mathbf{M}} f dx = \sum_{\xi_k \in M_\rho} \mu_{\xi_k} f(\xi_k).$$

Moreover, there exists constants c_1, c_2 , such that the following inequalities hold:

$$(24) \quad c_1 \rho^n \leq \mu_{\xi_k} \leq c_2 \rho^n, \quad n = \dim \mathbf{M}.$$

9.2. On the product of eigenfunctions of the Casimir operator \mathcal{L} on compact homogeneous manifolds. A *homogeneous* compact manifold \mathbf{M} is a C^∞ -compact manifold on which a compact Lie group G acts transitively. In this case \mathbf{M} is necessarily of the form G/K , where K is a closed subgroup of G . The notation $L_2(\mathbf{M})$, is used for the usual Hilbert spaces $L_2(\mathbf{M}, d\xi)$, where $d\xi$ is an invariant measure.

Every element X of the (real) Lie algebra of G generates a vector field on \mathbf{M} , which we will denote by the same letter X . Namely, for a smooth

function f on \mathbf{M} one has

$$Xf(\xi) = \lim_{t \rightarrow 0} \frac{f(\exp tX \cdot \xi) - f(\xi)}{t}$$

for every $\xi \in \mathbf{M}$. In the future we will consider on \mathbf{M} only such vector fields. The translations along integral curves of such vector fields X on \mathbf{M} can be identified with a one-parameter group of diffeomorphisms of \mathbf{M} , which is usually denoted as $\exp tX$, $-\infty < t < \infty$. At the same time, the one-parameter group $\exp tX$, $-\infty < t < \infty$, can be treated as a strongly continuous one-parameter group of operators acting on the space $L_2(\mathbf{M})$. These operators act on functions according to the formula

$$f \rightarrow f(\exp tX \cdot \xi), \quad t \in \mathbb{R}, \quad f \in L_2(\mathbf{M}), \quad x \in \mathbf{M}.$$

The generator of this one-parameter group will be denoted by D_X , and the group itself will be denoted by

$$e^{tD_X} f(\xi) = f(\exp tX \cdot \xi), \quad t \in \mathbb{R}, \quad f \in L_2(\mathbf{M}), \quad \xi \in \mathbf{M}.$$

According to the general theory of one-parameter groups in Banach spaces, the operator D_X is a closed operator on every $L_2(\mathbf{M})$.

If \mathfrak{g} is the Lie algebra of a compact Lie group G then ([12], Ch. II,) it is a direct sum $\mathfrak{g} = \mathfrak{a} + [\mathfrak{g}, \mathfrak{g}]$, where \mathfrak{a} is the center of \mathfrak{g} , and $[\mathfrak{g}, \mathfrak{g}]$ is a semi-simple algebra. Let Q be a positive-definite quadratic form on \mathfrak{g} which, on $[\mathfrak{g}, \mathfrak{g}]$, is opposite to the Killing form. Let X_1, \dots, X_d be a basis of \mathfrak{g} , which is orthonormal with respect to Q . Since the form Q is $Ad(G)$ -invariant, the operator

$$-X_1^2 - X_2^2 - \dots - X_d^2, \quad d = \dim G,$$

is a bi-invariant operator on G . This implies in particular that the corresponding operator on $L_2(\mathbf{M})$

$$(25) \quad \mathcal{L} = -D_1^2 - D_2^2 - \dots - D_d^2, \quad D_j = D_{X_j}, \quad d = \dim G,$$

commutes with all operators $D_j = D_{X_j}$.

This elliptic second order differential operator \mathcal{L} is usually called the Laplace operator. In the case of a compact semi-simple Lie group, or a compact symmetric space of rank one the operator \mathcal{L} is, or is proportional to, the Laplace-Beltrami operator of an invariant metric on \mathbf{M} .

The following theorem was proved in [11], [25].

Theorem 16. *If $\mathbf{M} = G/K$ is a compact homogeneous manifold and \mathcal{L} is defined as in (25), then for any f and g belonging to $\mathbf{E}_\omega(\mathcal{L})$, their product fg belongs to $\mathbf{E}_{4d\omega}(\mathcal{L})$, where d is the dimension of the group G .*

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